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M a t h e m a t i c s

MOORE–PENROSE INVERSE OF BIDIAGONAL MATRICES. IV

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The present work completes a research started in the papers [1–3]. Based on the results obtained in the previous papers, here we give a definitive solution to the problem of the Moore–Penrose inversion of singular upper bidiagonal matrices.

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Introduction. We consider a problem of the Moore–Penrose inversion of singular upper bidiagonal matrices

$$A = \begin{bmatrix} d_1 & b_1 & & & \\ & d_2 & b_2 & 0 & \\ & & \ddots & \ddots & \\ & 0 & & d_{n-1} & b_{n-1} \\ & & & & d_n \end{bmatrix} \tag{1}$$

under the assumption $b_1, b_2, \ldots, b_{n-1} \neq 0$ (note that this assumption does not restrict the generality of the problem, since if some of over-diagonal entries of the matrix A are zero, then the original problem is decomposed into several similar problems for bidiagonal matrices of lower order). In [1] we obtained a solution to the problem in a special case, where $d_1, d_2, \ldots, d_{n-1} \neq 0$, $d_n = 0$.

To solve the problem for any arrangement of one or more zeros on the main diagonal of the matrix A, in [2, 3] we carried out some preliminary constructions and calculations. At first, we represented the matrix (1) in the block form

$$A = \begin{bmatrix} A_1 & B_1 & & & \\ & A_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & A_{m-1} & B_{m-1} \\ & & & & A_m \end{bmatrix} \tag{2}$$

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with diagonal blocks A_k, $k = 1,2,\ldots,m$, of the size $n_k \times n_k$ and over-diagonal blocks B_k, $k = 1,2,\ldots,m-1$, of the size $n_k \times n_{k+1}$, where $n_1 + n_2 + \cdots + n_m = n$. The structure of the blocks was specified in the **Introduction** of [2]; ibid the types 1, 2 and 3 of the blocks A_k have been identified. Note that by virtue of the partitioning rule, only the last block A_m in (2) can be a block of type 3. The blocks B_k are given in (5) of [2].

As has been shown in [2] (see **A Way of Computing the Moore–Penrose Invertion**), the matrix A^+ has the following block form:

$$A^+ = \begin{bmatrix} Z_1 & & & & & \\ H_2 & Z_2 & & & 0 & \\ & \ddots & \ddots & & & \\ & 0 & H_{m-1} & Z_{m-1} & & \\ & & & H_m & Z_m \end{bmatrix}; \tag{3}$$

the blocks Z_k and H_k are computed by the formulae

$$Z_k = \lim_{\varepsilon\to+0} L_k(\varepsilon)^{-1} A_k^T, \quad k = 1,2,\ldots,m, \tag{4}$$

$$H_k = \lim_{\varepsilon\to+0} L_k(\varepsilon)^{-1} B_{k-1}^T, \quad k = 2,3,\ldots,m, \tag{5}$$

where

$$L_1(\varepsilon) = A_1^T A_1 + \varepsilon I_1, \tag{6}$$

$$L_k(\varepsilon) = A_k^T A_k + B_{k-1}^T B_{k-1} + \varepsilon I_k, \quad k = 2,3,\ldots,m, \tag{7}$$

and I_k stands for the identity matrix of the order n_k.

For the purpose of simplifying the record of subsequent formulae, let us write the block A_k, $1 \le k \le m$, in the form

$$A_k = \begin{bmatrix} d_1^{(k)} & b_1^{(k)} & & & \\ & d_2^{(k)} & b_2^{(k)} & 0 & \\ & & \ddots & \ddots & \\ & 0 & & d_{n_k-1}^{(k)} & b_{n_k-1}^{(k)} \\ & & & & d_{n_k}^{(k)} \end{bmatrix}, \tag{8}$$

where, according to (1),

$$\begin{aligned} d_i^{(k)} &= d_{n_1+\cdots+n_{k-1}+i}, \quad i = 1,2,\ldots,n_k, \\ b_i^{(k)} &= b_{n_1+\cdots+n_{k-1}+i}, \quad i = 1,2,\ldots,n_k-1. \end{aligned} \tag{9}$$

We introduce the following notation:

$$r_s^{(k)} = \frac{b_s^{(k)}}{d_s^{(k)}}, \ s = 1,2,\ldots,n_k-1; \ r_0^{(k)} = r_{n_k}^{(k)} = 1. \tag{10}$$

Further, let

$$\Delta_k = b_{n_1+n_2+\cdots+n_k}, \ k = 1,2,\ldots,m-1 \tag{11}$$

(see (5) in [2]).

Based on the results obtained in the previous articles [1–3], below we give a closed form expressions for the entries of the matrix A^+ as well as a numerical algorithm for their computation.

Computation of the Blocks Z_k. Let us start with the block Z_1. The problem of computing this block was discussed in [2] (see **Block** Z_1). If the corresponding block A_1 is of type 1, then the entries of the block $Z_1 = A_1^+$ are computed using the formulae (50)–(52) from [1]. If A_1 is a block of type 2, then $Z_1 = [0]_{1\times 1}$ for $n_1 = 1$; for $n_1 \geq 2$ the block Z_1 is the lower bidiagonal matrix given in (17) of [2].

Note that if $m = 1$ (see the block representation (3) of the matrix A), then obviously $A^+ = Z_1$.

Let us discuss the blocks Z_k, $2 \leq k \leq m$. If A_k is a block of type 1, the formulae for the entries of the block Z_k are actually obtained in Lemma 3 of [3] (replacing n with n_k and taking into account notation (9),(10)). If A_k is a block of type 2, the entries of the block Z_k are derived in Lemma 5 of [3] (replacing n with n_k and using notation (9)). As has been said above, only the last block A_m in (2) can be a block of type 3. In this case the entries of the block Z_m are computed by the formulae derived in Lemma 1 of [3] (replacing n with n_m, Δ with Δ_{m-1} and taking into account notation (9),(10)).

Thus, we arrive at to the following statement.

Theorem 1. Let a singular upper bidiagonal matrix A from (1) with non-zero over-diagonal entries is represented in the block form (2), according to the rule described in **Introduction** of [2]. Then the entries of diagonal blocks $Z_k = [z_{ij}^{(k)}]_{n_k \times n_k}$, $1 \leq k \leq m$, in the block representation (3) of the matrix A^+ are computed as follows.

I. The entries of the block Z_1:

1) if A_1 is a block of type 1, then

1a) for the indeces $j = 1,2,\ldots,n_1-1$ and $i = 1,2,\ldots,j$:

$$z_{ij}^{(1)} = \frac{(-1)^{i+j}\displaystyle\sum_{k=1}^{n_1-j}\left(\prod_{s=j}^{n_1-k}\frac{1}{r_s^{(1)}}\right)\left(\prod_{s=n_1-k+1}^{n_1-1} r_s^{(1)}\right)}{\displaystyle\prod_{s=1}^{i-1} r_s^{(1)}\cdot d_j^{(1)}\sum_{k=1}^{n_1}\left(\prod_{s=1}^{n_1-k}\frac{1}{r_s^{(1)}}\right)\left(\prod_{s=n_1-k+1}^{n_1-1} r_s^{(1)}\right)};$$

1b) for the indeces $j = 1,2,\ldots,n_1-1$ and $i = j+1, j+2,\ldots,n_1$:

$$z_{ij}^{(1)} = \frac{(-1)^{i+j+1}\left(\displaystyle\prod_{s=i}^{n_1-1} r_s^{(1)}\right)\cdot\sum_{k=1}^{j}\left(\prod_{s=1}^{k-1}\frac{1}{r_s^{(1)}}\right)\left(\prod_{s=k}^{j-1} r_s^{(1)}\right)}{d_j^{(1)}\displaystyle\sum_{k=1}^{n_1}\left(\prod_{s=1}^{n_1-k}\frac{1}{r_s^{(1)}}\right)\left(\prod_{s=n_1-k+1}^{n_1-1} r_s^{(1)}\right)};$$

1c) for the index $j = n_1$:

$$z_{in_1}^{(1)} = 0, \quad i = 1,2,\ldots,n_1;$$

2) if A_1 is a block of type 2, then

for $n_1 = 1$:

$$Z_1 = [0]_{1\times 1};$$

for $n_1 \geq 2$:

$$z_{i\,i-1}^{(1)} = \frac{1}{b_{i-1}^{(1)}}, \quad i = 2,3,\ldots,n_1,$$

$$z_{ij}^{(1)} = 0 \quad \text{in the remaining cases.}$$

II. The entries of the blocks $Z_k,\ 2 \le k \le m$:

3) if A_k is a block of type 1, then

3a) for the indeces $j = 1,2,\dots,n_k$ and $i = 1,2,\dots,j$:

$$z_{ij}^{(k)} = 0;$$

3b) for the indeces $j = 1,2,\dots,n_k - 1$ and $i = j+1, j+2,\dots,n_k$:

$$z_{ij}^{(k)} = \frac{(-1)^{i+j+1}}{d_j^{(k)}} \prod_{s=j}^{i-1} \frac{1}{r_s^{(k)}};$$

4) if A_k is a block of type 2, then

for $n_k = 1$:

$$Z_k = [0]_{1\times 1};$$

for $n_k \ge 2$:

$$z_{i\,i-1}^{(k)} = \frac{1}{b_{i-1}^{(k)}}, \quad i = 2,3,\dots,n_k,$$

$$z_{ij}^{(k)} = 0 \quad \text{in the remaining cases;}$$

5) if A_m is a block of type 3 and $n_m = 1$, then

$$Z_m = \left[\frac{d_1^{(m)}}{d_1^{(m)2} + \Delta_{m-1}^2} \right]_{1\times 1};$$

6) if A_m is a block of type 3 and $n_m \ge 2$, then

6a) for the indeces $j = 1,2,\dots,n_m$ and $i = 1,2,\dots,j$:

$$z_{ij}^{(m)} = \frac{(-1)^{i+j} \left[\prod_{s=1}^{i-1} \frac{1}{r_s^{(m)}} + \Delta_{m-1}^2 \sum_{k=1}^{i-1} \frac{1}{b_k^{(m)2}} \left(\prod_{s=1}^{k} r_s^{(m)} \right) \left(\prod_{s=k+1}^{i-1} \frac{1}{r_s^{(m)}} \right) \right] \kappa_j^{(m)}}{d_{n_m}^{(m)2} \left[\prod_{s=1}^{n_m-1} \frac{1}{r_s^{(m)}} + \Delta_{m-1}^2 \sum_{k=1}^{n_m-1} \frac{1}{b_k^{(m)2}} \left(\prod_{s=1}^{k} r_s^{(m)} \right) \left(\prod_{s=k+1}^{n_m-1} \frac{1}{r_s^{(m)}} \right) \right] + D^{(m)}},$$

where

$$\kappa_j^{(m)} \equiv \frac{d_{n_m}^{(m)2}}{d_j^{(m)}} \prod_{s=j}^{n_m-1} \frac{1}{r_s^{(m)}}, \quad D^{(m)} \equiv \Delta_{m-1}^2 \prod_{s=1}^{n_m-1} r_s^{(m)};$$

6b) for the indeces $j = 1,2,\dots,n_m - 1$ and $i = j+1, j+2,\dots,n_m$:

$$z_{ij}^{(m)} = \frac{(-1)^{i+j+1} \left[\prod_{s=i}^{n_m-1} r_s^{(m)} + d_{n_m}^{(m)2} \sum_{k=i}^{n_m-1} \frac{1}{d_k^{(m)2}} \left(\prod_{s=i}^{k-1} r_s^{(m)} \right) \left(\prod_{s=k}^{n_m-1} \frac{1}{r_s^{(m)}} \right) \right] \omega_j^{(m)}}{d_{n_m}^{(m)2} \left[\prod_{s=1}^{n_m-1} \frac{1}{r_s^{(m)}} + \Delta_{m-1}^2 \sum_{k=1}^{n_m-1} \frac{1}{b_k^{(m)2}} \left(\prod_{s=1}^{k} r_s^{(m)} \right) \left(\prod_{s=k+1}^{n_m-1} \frac{1}{r_s^{(m)}} \right) \right] + D^{(m)}},$$

where

$$\omega_j^{(m)} \equiv \frac{\Delta_{m-1}^2}{d_j^{(m)}} \prod_{s=1}^{j-1} r_s^{(m)}, \quad D^{(m)} \equiv \Delta_{m-1}^2 \prod_{s=1}^{n_m-1} r_s^{(m)}.$$

Thus, we have got the formulae to compute the entries of the blocks Z_k.

Computation of the Blocks H_k. Proceed to the blocks H_k, $2 \le k \le m$, in the block representation (3) of the matrix A^+. If A_k is a block of type 1, the entries of the corresponding block H_k are computed by the formulae derived in Lemma 4 of [3] (naturally, replacing n with n_k, l with n_{k-1}, Δ with Δ_{k-1} and taking into account notation (9),(10)). Further, if A_k is a block of type 2, the entries of the block H_k are computed according to Lemma 6 from [3] (replacing Δ with Δ_{k-1}). Finally, if A_m is a block of type 3, the entries of the block H_m are computed by the formulae derived in Lemma 2 of [3] (replacing n with n_m, l with n_{m-1}, Δ with Δ_{m-1} and taking into account notation (9),(10)).

As a result we get the following statement:

Theorem 2. Let a singular upper bidiagonal matrix A from (1) with non-zero over-diagonal entries is represented in the block form (2), according to the rule described in **Introduction** of [2]. Then the entries of under-diagonal blocks $H_k = [h_{ij}^{(k)}]_{n_k \times n_{k-1}}$, $2 \le k \le m$, in the block representation (3) of the matrix A^+ are computed as follows:

1) if A_k is a block of type 1, then

$$h_{i\,n_{k-1}}^{(k)} = \frac{(-1)^{i+1}}{\Delta_{k-1}} \prod_{s=1}^{i-1} \frac{1}{r_s^{(k)}}, \quad i = 1,2,\ldots,n_k,$$

$$h_{ij}^{(k)} = 0 \quad \text{in the remaining cases;}$$

2) if A_k is a block of type 2, then

$$h_{1\,n_{k-1}}^{(k)} = \frac{1}{\Delta_{k-1}},$$

$$h_{ij}^{(k)} = 0 \quad \text{in the remaining cases;}$$

3) if A_m is a block of type 3 and $n_m = 1$, then

$$h_{1\,n_{m-1}}^{(m)} = \frac{\Delta_{m-1}}{d_1^{(m)^2} + \Delta_{m-1}^2};\ h_{1j} = 0,\ j = 1,2,\ldots,n_{m-1}-1;$$

4) if A_m is a block of type 3 and $n_m \ge 2$, then

4a) for the indeces $j = 1,2,\ldots,n_{m-1}-1$ and $i = 1,2,\ldots,n_m$:

$$h_{ij}^{(m)} = 0;$$

4b) for the indeces $j = n_m$ and $i = 1,2,\ldots,n_m$:

$$h_{i n_{m-1}}^{(m)} = \frac{(-1)^{i+1}\Delta_{m-1}\left[\prod\limits_{s=i}^{n_m-1} r_s^{(m)} + d_{n_m}^{(m)^2} \sum\limits_{k=i}^{n_m-1} \frac{1}{d_k^{(m)^2}} \left(\prod\limits_{s=i}^{k-1} r_s^{(m)}\right)\left(\prod\limits_{s=k}^{n_m-1} \frac{1}{r_s^{(m)}}\right)\right]}{d_{n_m}^{(m)^2}\left[\prod\limits_{s=1}^{n_m-1} \frac{1}{r_s^{(m)}} + \Delta_{m-1}^2 \sum\limits_{k=1}^{n_m-1} \frac{1}{b_k^{(m)^2}} \left(\prod\limits_{s=1}^{k} r_s^{(m)}\right)\left(\prod\limits_{s=k+1}^{n_m-1} \frac{1}{r_s^{(m)}}\right)\right] + D^{(m)}},$$

where $D^{(m)} \equiv \Delta_{m-1}^2 \prod\limits_{s=1}^{n_m-1} r_s^{(m)}$.

Thus, in Theorems 1 and 2 we have derived closed form expressions for the entries of the Moore–Penrose inverse of upper bidiagonal matrix A from (1). In the next section we discuss an issue of practical computation of the matrix A^+.

A Procedure to Compute the Moore–Penrose Inverse. In the paper [2] we have developed a computational procedure of finding the first diagonal block Z_1 in the block representation (3) of the matrix A^+ (see **Block** Z_1, Procedure **Z1**). Further, in the paper [3] we have developed numerical algorithms to compute model matrices Z and H (see (10),(11) in [3]). Taking advantage of these results, below we give the following computational procedure.

Procedure 2d/pinv $(A, n \Rightarrow A^+)$

Input: an upper bidiagonal matrix A of the form (1).

1. A partition (2) of the matrix A into blocks according to the rule specified in [2](**Introduction**); identification of the blocks A_k $(1 \le k \le m)$, $B_k(1 \le k \le m-1)$ and determination of the parameters n_k, $1 \le k \le m$, which define the block sizes. In each block A_k its own internal numbering of the entries is given (see (8),(9)). The quantities Δ_k, $1 \le k \le m-1$, are introduced (see (11)).
2. The block Z_1 in the block representation (3) of the matrix A^+ is computed. For that the procedure **Z1** $(A_1, n_1 \Rightarrow Z_1)$ from [2] is used. The procedure requires $n_1^2 + O(n_1)$ arithmetical operations.
   If $m = 1$, then the computations are completed and $A^+ = Z_1$.
   If $m \ge 2$, then proceed to successive computation of the blocks Z_k and H_k, for $k = 2, 3, \ldots, m$.
3. If A_k is a block of type 1, the blocks Z_k and H_k are computed using the algorithm **Z,H/caseB** $(A_k, \Delta_{k-1}, n_k, n_{k-1} \Rightarrow Z_k, H_k)$ given in [3]. The algorithm requires $(1/2)n_k^2 + O(n_k)$ arithmetical operations.
4. If A_k is a block of type 2, simple expressions for the entries of the blocks Z_k and H_k are obtained in Lemmas 5 and 6 of [3]:

   if $n_k = 1$, then

$$Z_k = [0]_{1\times 1}, \quad H_k = \left[0 \ldots 0 \, \frac{1}{\Delta_{k-1}} \right]_{1\times n_{k-1}};$$

   if $n_k \ge 2$, then

$$Z_k = \begin{bmatrix} 0 & & & & \\ b_1^{(k)^{-1}} & 0 & & 0 & \\ & b_2^{(k)^{-1}} & 0 & & \\ & 0 & \ddots & \ddots & \\ & & & b_{n_k-1}^{(k)^{-1}} & 0 \end{bmatrix}, \quad H_k = \begin{bmatrix} 0 & 0 & \ldots & 0 & \frac{1}{\Delta_{k-1}} \\ 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 0 \end{bmatrix}.$$

   It requires no more than n_k arithmetical operations.
5. If A_m is a block of type 3, the blocks Z_m and H_m are computed using the algorithm **Z,H/caseA** $(A_m, \Delta_{m-1}, n_m, n_{m-1} \Rightarrow Z_m, H_m)$ given in [3]. The algorithm requires $n_m^2 + O(n_m)$ arithmetical operations.

Output: matrix A^+.

End procedure

Direct calculations show that for $m \geq 2$ the described computational procedure requires no more than

$$n_1^2 + \frac{1}{2}\sum_{k=2}^{m-1} n_k^2 + n_m^2 + O(n)$$

arithmetical operations (recall that $n_1 + n_2 + \cdots + n_m = n$). If $m = 1$, this number does not exceed $n_1^2 + O(n_1)$.

Thus we can formulate the following statement.

Proposition. Let A be a singular upper bidiagonal matrix of the form (1) with non-zero over-diagonal entries $b_1, b_2, \ldots, b_{n-1}$. Then the Moore–Penrose inverse A^+ of this matrix can be obtained using the computational procedure **2d/pinv**, which requires no more than $n_1^2 + O(n_1)$ (if $m = 1$) or $n_1^2 + \frac{1}{2}\sum_{k=2}^{m-1} n_k^2 + n_m^2 + O(n)$ (if $m \geq 2$) arithmetical operations.

As a clarification, we note the following important features of the procedure. Proceeding from the structure of the blocks in the block representation (3) of the matrix A^+ (namely, the presence of zeros located at predetermined places) and estimation of the number of arithmetical operations required to compute each block, we can assert that for computing one non-zero entry of the matrix A^+ asymptotically is expended one arithmetical operation. Thereby the proposed method can be considered as an optimal.

Concluding Remarks. As a result of the study carried out we have obtained a solution to the problem of the Moore–Penrose inverstion of singular upper bidiagonal matrices. We have derived a closed form expressions for the entries of pseudoinverse matrix and developed an optimal numerical algorithm for their computation.

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